E1 transitions in Ni II

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Abstract. We have undertaken an extensive CI calculation of E1 transitions between all levels of the 3d⁹, 3d⁸4s, 3d⁷4s² and 3d⁸4p, 3d⁷4s4p configurations of Ni II. Many of these lines are observed in a variety of astronomical objects, and so atomic data is needed, with a good level of accuracy, for the analysis of the observational data. To date, only a limited number of extensive calculations have been undertaken for this ion [1,2] while experimental [3,4,5] or observationally derived [6,7] atomic data are limited to an even smaller selection of lines.

In this work, we have used the general CI code CIV3 [8] in which relativistic effects are incorporated using the Breit-Pauli approximation. In addition, *ab initio* results are enhanced by our fine-tuning process which seeks to bring the calculated energy levels into line with experimental levels.

For many of the lines studied, our results are in good agreement with those of [1,2]. But it is not always so. This is illustrated below for oscillator strengths (length form) of a very small selection of 4s – 4p lines, with a common lower level.

Transition	Oscillator strengths		
	This work	[1]	[2]
$3d^{8}(^{3}P)4s^{2}P_{0.5}^{o} - 3d^{8}(^{3}P)4p^{2}P_{1.5}^{o}$ $3d^{8}(^{3}P)4s^{2}P_{0.5}^{o} - 3d^{8}(^{1}D)4p^{2}P_{1.5}^{o}$	0.0870	0.2264	0.2511
$3d^{8}(^{3}P)4s^{2}P_{0.5}^{00} - 3d^{8}(^{1}D)4p^{2}P_{1.5}^{00}$	0.0602	0.0321	0.0271
$3d^{8}(^{3}P)4s^{2}P_{0.5}^{o} - 3d^{8}(^{3}P)4p^{2}D_{1.5}^{o}$	0.3904	0.3062	0.3008
$3d^{8}(^{3}P)4s^{2}P_{0.5}^{00} - 3d^{8}(^{3}P)4p^{4}S_{1.5}^{00}$	0.0098	0.0035	0.0002
Total	0.5474	0.5682	0.5782

so, although the total of the four f-values is almost the same, there is a significant variation in the distribution of the oscillator strength, due to different CI mixings in the upper levels. For example, for the $3d^8(^3P)4p$ $^2P^o_{1.5}$ level, the main percentage compositions are

$$\begin{array}{ll} Our\ work & 45\%(3d^8(^3P)4p\ ^2P_{1.5}^o) + 29\%(3d^8(^1D)4p\ ^2P_{1.5}^o) + 14\%(3d^8(^3P)4p\ ^4S_{1.5}^o) \\ Kurucz & 69\%(3d^8(^3P)4p\ ^2P_{1.5}^o) + 15\%(3d^8(^1D)4p\ ^2P_{1.5}^o) + 9\%(3d^8(^3P)4p\ ^2D_{1.5}^o) \end{array}$$

Further results and discussion will be presented at the conference.

REFERENCES

- 1. R. L. Kurucz, http://kurucz.harvard.edu/atoms.html (Ni II), (2000).
- 2. S. Fritzsche, C. Z. Dong, and G. Gaigalas, Atom. Data Nucl. Data Tables 76, 155–170 (2000).
- 3. F. S. Ferrero, J. Manrique, M. Zwegers, and J. Campos, *J. Phys. B: At. Mol. Opt. Phys.* **30**, 893–903 (1997).
- 4. J. A. Fedchak, and J. E. Lawler, Ap. J. 523, 734–738 (1999).
- 5. J. A. Fedchak, L. M. Wiese, and J. E. Lawler, Ap. J. **538**, 773–776 (1999).
- 6. J. Zsargo, and S. R. Federman, Ap. J. 498, 256–260 (1998).
- 7. E. B. Jenkins, and T. M. Tripp, Ap. J. 637, 548–552 (2006).
- 8. A. Hibbert, *Comp. Phys. Commun.* **9**, 141–172 (1975); A. Hibbert, R. Glass, and C. F. Fischer, *Comp. Phys. Commun.* **64**, 455-472 (1991).